We claim:

1.   A computer system for calculating a pharmacokinetic behavior of a chemical substance in an insect, comprising:

- a physiologically based pharmacokinetic simulation model (102) of said insect for predicting concentration/time profiles of the chemical substance in compartments of the insect, the simulation model having at least one parameter which is dependent on the substance,

- a prediction module (110) for predicting the at least one parameter on the basis of a physicochemical property of the substance.

2.   Computer system according to Claim 1, wherein the at least one parameter is the product of the permeability for the substance and the effective surface area of the compartments.

3.   Computer system according to Claim 1, wherein said at least one parameter is the rate coefficient for inter-compartmental mass transport ($\lambda_x = P A_x/V_x$), the volume of at least one of the organs of the insect being a function of time ($V_x = V_x(t)$).

4.   Computer system according to Claim 1, wherein said at least one parameter is the equilibrium coefficient between an organ of the insect and the haemolymph (K_x, $x \in \{c, mu, fb, nc$ and $gw\}$), between the surface of the cuticle and the cuticle ($K_{c/cs}$), or between the gut wall and the gut content ($K_{gc/gw}$).

5.   Computer system according to Claim 1, wherein said physicochemical property is the distribution coefficient between water and phospholipid membranes, the octanol/water distribution coefficient, the molecular weight, the solubility, and/or a combination of these parameters of the substance.

6.   Computer system according to Claim 1, comprising a QSAR model or a neural network for determining the physicochemical property from a descriptor of the chemical structure of the substance.

7.   Computer system according to Claim 1, wherein the prediction module is based on a database (108) which contains the physicochemical properties of test substances and parameters determined experimentally for the test substances.

8.   Computer system according to Claim 1, wherein the prediction module includes a calculation function for calculating said at least one parameter from the lipophilicity and/or the molecular weight of the substance.

9.   Computer system according to Claim 8, wherein the calculation function is based on a linear regression of experimentally determined parameter values.

10.   Method for calculating a pharmacokinetic behavior of a chemical substance in insects, using a physiologically based pharmacokinetic simulation model of an insect for predicting concentration/time profiles of the chemical substance in compartments of the insect, the simulation model having at least one parameter which is dependent on the substance, comprising the following steps:

- input of a physicochemical property of the substance into a prediction module for predicting the at least one parameter for the substance,

- carrying out a simulation with the simulation model for predicting concentration/time profiles of the chemical substance on the basis of the predicted at least one parameter.

11.   Method according to Claim 10, wherein said at least one parameter is the product of the permeability of the compartments of the insect to the substance and the effective surface area of the compartments.

12.   Method according to Claim 10, wherein the parameter is the rate coefficient for inter-compartmental mass transport ($\lambda_x = P_x A_x/V_x$), the volume of at least one of the organs of the insect being a function of time ($V_x = V_x(t)$).

13.   Method according to Claim 10, wherein the parameter is the equilibrium coefficient between an organ and the haemolymph (K_x, $x \in \{c, mu, fb, nc$ and $gw\}$), between the surface of the cuticle and the cuticle ($K_{c/cs}$), or between the gut wall and the gut content ($K_{gc/gw}$).

14.   Method according to Claims 10, wherein the physicochemical property is the distribution coefficient between water and phospholipid membranes, the octanol/water distribution coefficient, the molecular weight, the solubility, and/or a combination of these parameters of the substance.

15.   Method according to Claim 10, wherein the physicochemical property is determined by a QSAR model or a neural network.

16.   Method according to Claim 10, wherein the prediction of the at least one parameter is based on physicochemical properties of test substances and parameter values determined experimentally for the test substances.

17.   Method according to Claim 10, wherein the prediction of the at least one parameter is carried out with a calculation function from the lipophilicity and/or the molecular weight of the substance.

18.   Method according to Claim 10, wherein the calculation function isbased on a linear regression of experimentally determined parameter values.

19.   A digital storage mediumhaving stored thereon a program for calculating a pharmacokinetic behavior of a chemical substance in insects with a physiologically based pharmacokinetic simulation model of an insect for predicting concentration/time profiles of the chemical substance in compartments of the insect, the simulation model having at least one parameter which is dependent on the substance, with the following steps:

- input of a physicochemical property of the substance into a prediction module for predicting the at least one parameter for the substance,

- carrying out a simulation with the aid of the simulation model for predicting concentration/time profiles of the chemical substance one the basis of the predicted at least one parameter.

20.   Digital storage medium according to Claim10, wherein said at least one parameter is the product of the permeability for the substance and the effective surface area of the compartments.

21.   Digital storage medium according to Claim 19, wherein said at least one parameter is the rate coefficient for inter-compartmental mass transport $(\lambda_x = P_x A_x/V_x)$, the volume (V_x) of at least one of the organs of the insect being a function of time $(V_x = V_x(t))$.

22.   Digital storage medium according to Claim 19, wherein said at least one parameter is the equilibrium coefficient between an organ and the haemolymph $(K_x, x \in \{c, mu, fb, nc$ and $gw\})$, between the surface of the cuticle and the cuticle $(K_{c/cs})$, or between the gut wall and the gut content $(K_{gc/gw})$.

23.   Digital storage medium according to Claim 19, wherein said physico-chemical property is the distribution coefficient between water and phospholipid membranes, the octanol/water distribution coefficient, the molecular weight, the solubility, and/or a combination of these parameters of the substance.

24.   Digital storage medium according to Claim 19, having further stored thereon, separately or as part of said program, a QSAR model or a neural network for determining said physicochemical property from a descriptor of the chemical structure of the substance.

25.   Digital storage medium according to Claim 19, wherein said prediction module is based on a database (108) which contains the physicochemical properties of test substances and parameters determined experimentally for the test substances.

26.   Digital storage medium according to Claim 29, wherein said prediction module comprises a calculation function for calculating the parameters from the lipophilicity and/or the molecular weight of the substance.

27.   Digital storage medium according toClaim 26, wherein said calculation function is based on a linear regression of experimentally determined parameter values.